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13. ABSTRACT *(Maximum 200 Words)*

Work completed, or in progress, by the end of the first grant year includes a study of the effects of initial conditions on high Reynolds number shear layers, where it was shown that they also influence molecular mixing far downstream of the splitter plate; moderate Reynolds number, liquid-phase transverse jets in a cross flow, including their three-dimensional structure; the discovery of a power-law similarity in the surface-to root-area ratio of scalar structures in liquid-phase turbulent jets; numerical investigations of hydrocarbon ignition and the effects of additives in a high-strain rate environment, as would be encountered in air-breathing scramjet propulsion; and further advances and applications of velocity-field measurements from image sequences of convected scalars.

14. SUBJECT TERMS
Turbulence, turbulent mixing, chemical-reacting flows, combustion, supersonic flow, level sets, hypersonic

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Mixing, chemical reactions, and combustion in subsonic and supersonic turbulent flows

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Summary and status overview

This effort is focused on fundamental investigations of mixing, chemical-reaction, and combustion processes, in turbulent, subsonic, and supersonic free-shear flows. The program is comprised of an experimental effort; an analytical, modeling, and computational effort; and a diagnostics and data-acquisition-development effort. The computational studies are focused on fundamental issues pertaining to the hydrocarbon-ignition/-combustion and numerical simulation of compressible flows with strong fronts, in both chemically-reacting and nonreacting flows.

1. Accomplishments and new findings

To investigate the effects of various parameters on turbulent-shear-layer mixing and combustion at high Reynolds number, experiments were conducted to explore the influence of inflow conditions. Chemically-reacting, incompressible, shear-layer flows were investigated in the GALCIT Supersonic Shear Layer Facility, at freestream conditions $U_2/U_1 \simeq 0.4$ and $\rho_2/\rho_1 \simeq 1$ and a local Reynolds number, $Re_\delta \equiv \rho \Delta U \delta(x)/\mu \sim 2 \times 10^5$.

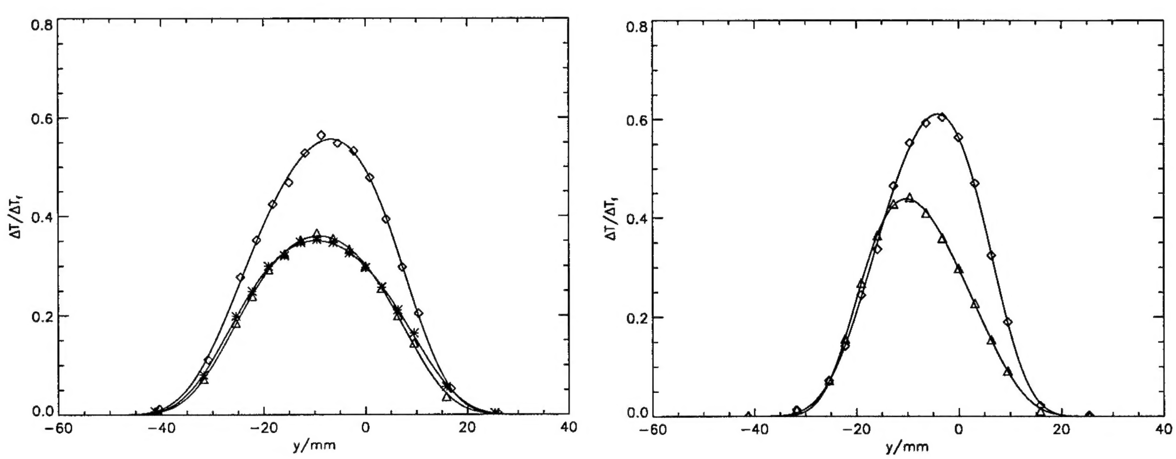

FIG. 1 Normalized temperature-rise data. Left: untripped boundary layers. Right: tripped high-speed boundary layer. Reactant compositions - diamonds: $\phi = 8$; triangles: $\phi = 1/8$; asterisks: $\phi = 1/8$, reduced chemical-kinetic rate.

Chemically-reacting "flip" experiments allow us to deduce the structure and amount of molecular-scale mixing, information unobtainable from direct scalar imaging at such high Reynolds numbers. Two sets of temperature-rise data from such experiments are presented in Fig. 1. The only difference between these is a 0.8 mm-diameter trip wire on the splitter plate (high-speed side), 50 mm upstream of its trailing edge. The data are measured far downstream, at $x/\theta_1 \simeq 3300$, where x is the streamwise coordinate and θ_1 is the high-speed boundary layer momentum thickness, and at a large value of the pairing parameter,[1] $P \simeq 47$. By these criteria, the flow may be regarded as fully-developed.[2,3] The change in inflow conditions can be seen to have a significant effect on all scales of the flow: the shear-layer growth rate, δ/x, has decreased by 21%; the mixed-fluid fraction (efficiency of molecular-scale mixing), has increased by 11%; and the mixed-fluid composition ratio has decreased by 9%. Additionally, the data indicate a change from a non-marching scalar probability-density function (pdf), to a marching pdf, when the boundary layer was tripped. These observations suggest a shear-layer behavior that depends not only on local-flow properties, but also on upstream conditions, reminiscent of results from low-dimensionality, nonlinear (chaotic) systems.[4]

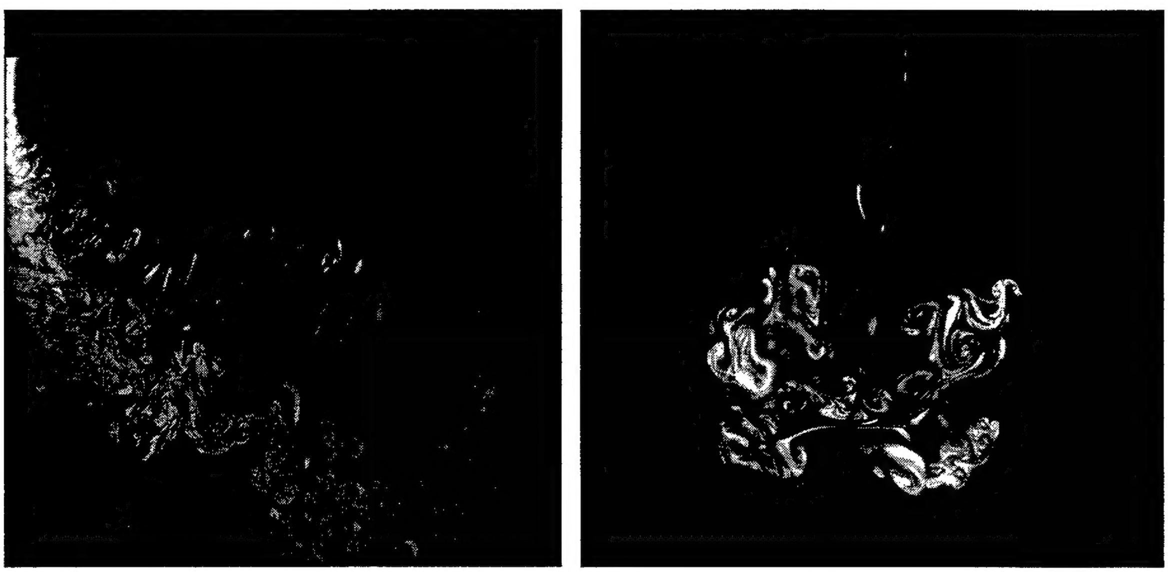

FIG. 2 Transverse jet at $Re_{\mathrm{j}} \simeq 1.0 \times 10^3$ and $U_{\mathrm{j}}/U_\infty \simeq 34$. Left: LIF image in plane parallel to free-stream (log-intensity scale). Right: Slice perpendicular to free-stream.

Experiments on the development and far-field structure of a liquid-phase turbulent jet issuing into a cross-flowing uniform stream were conducted at a jet Reynolds number, $Re_{\mathrm{j}} \equiv U_{\mathrm{j}} d_{\mathrm{j}}/\nu \simeq 1.0 \times 10^3$, for a velocity ratio, $U_{\mathrm{j}}/U_\infty \simeq 34$. Laser-induced fluorescence (LIF) images measured scalar-species concentration in two orthogonal

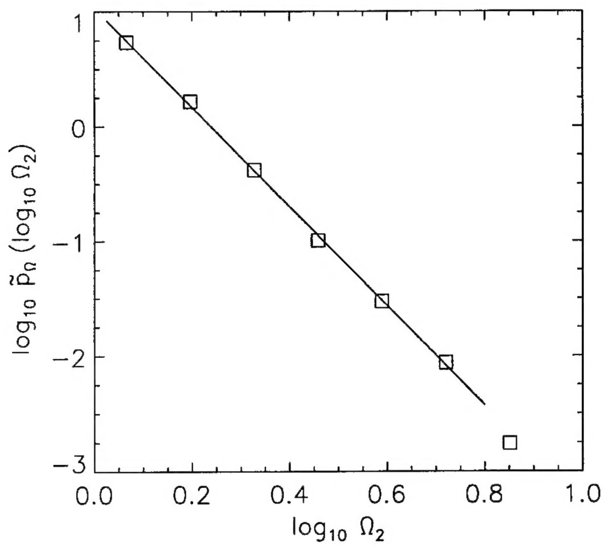

FIG. 3 Shape complexity pdf of islands and lakes. Solid line: power-law fit (in these coordinates).

slices of the transverse jet (Fig. 2). The data show wake structures similar to those reported previously,[5] *e.g.*, "fingers" of dyed jet-fluid extending from the tunnel wall to the main body of the jet. These are transported downstream with nearly uniform velocity after being formed near the jet exit.

As part of our investigation of the geometry of scalar isosurfaces in liquid-phase turbulent jets, an analysis of area-perimeter properties of isoscalar "islands" and "lakes" derived from 2-D images of jet-fluid concentration images has been conducted. The images are slices in a plane normal to the jet axis in the far field and correspond to a fluid Schmidt number of $Sc \simeq 2.0 \times 10^3$ and flow Reynolds numbers of $Re \simeq 4.5 \times 10^3$, 9.0×10^3, and 18×10^3.[6,7] For such data, scalar level sets form disjoint "islands" and "lakes", depending on whether the interior is at a lower, or higher, scalar level, respectively. Island/lake statistics, such as size and shape complexity, are important in many contexts: for chemical reactions and combustion in nonpremixed hydrocarbon turbulent flames, for example, combustion is largely confined to the instantaneous stoichiometric (isoscalar) surface.[8] In 2-D, such a measure, Ω_2, dubbed *shape complexity*, can be defined as,

$$1 \leq \Omega_2 \equiv \frac{P}{2\,(\,\pi A\,)^{1/2}} \leq \infty \,,$$

with P the perimeter and A an island/lake area, and $(\Omega_2)_{\min} = 1$ attained for a circle. Corresponding extensions can also be made for higher-dimensional embedding spaces.

Analysis of the liquid-phase jet data described above indicates that a power law for over 3 decades in size (6 decades in area), or, equivalently, log-Poisson statistics, provides a good approximation for the pdf of shape complexity, with similar behavior expected in turbulent flows in general. Such distributions are necessary in modeling burning-time distributions in nonpremixed combustion, for example.[9]

Numerical-simulation investigations were conducted on the ignition characteristics of hydrocarbon fuel blends, at conditions relevant to high-Mach-number, air-breathing-propulsion vehicles. A two-point-continuation method was employed, with a detailed description of molecular transport and chemical kinetics, focusing on the effects of fuel composition, reactant temperature, additives, and imposed strain rate. It captured the entire S-curve that describes the processes of vigorous burning, extinction, and ignition. The results demonstrate that ignition of such fuel blends is dominated by the synergistic behavior of CH_4 and C_2H_4. A fuel temperature $T_{\mathrm{fuel}} = 950\,\mathrm{K}$ was used in the simulations. For low air temperatures, *e.g.*, $T_{\mathrm{air}} \simeq 1050\,\mathrm{K}$, addition of small amounts of CH_4 enhances C_2H_4 ignition, while for $T_{\mathrm{air}} > 1200\,\mathrm{K}$, CH_4 inhibits ignition. The ignition of blends of CH_4 and C_2H_4 was significantly promoted through independent additions of small amounts of H_2, and F_2 with NO. The latter yields F-radicals which effectively consume hydrocarbon molecules. An important finding of these continuing investigations is that the GRI 2.1 C_1, C_2 kinetics mechanism, which was developed to describe CH_4 combustion, cannot represent ethylene (C_2H_4) ignition and kinetics. Interestingly, it is missing a key species, absent which, the strain rate sufficient to prevent ignition is underestimated by a factor of 25-30. A first report of this work was presented at the recent International Combustion Symposium (Boulder, CO).[10]

Developments on Image Correlation Velocimetry (ICV), a method that extracts velocity-field information from sequences of images of a convected scalar,[11,12] are continuing. This has been used to analyze two-dimensional slices of low-speed liquid-phase flows, with both particles and fluorescent dyes, as well as spacecraft imaging of the Jovian atmosphere. An important extension to a three-dimensional implementation is presently in progress, with envisaged initial testing on existing three-dimensional laboratory data on turbulent jets (*e.g.*, Ref. 13), as well as a variety of direct numerical-simulation (DNS) data. An application to Ozone Tagging Velocimetry image data,[14] is also in progress, in collaboration with R. W. Pitz and his group at Vanderbilt University, who are developing this technology. Finally, in collaboration with C. M. Vagelopoulos and F. N. Egolfopoulos (USC), an extension of the original particle-streak velocimetry technique,[15] targeted for strained flames and hydrocarbon laminar flame-speed measurement applications.

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3. Personnel

3.1 Personnel supported by this effort

- Catrakis, H. J., Assistant Scientist, Aeronautics. Presently, Assistant Professor, Mechanical and Aerospace Engineering, U. C. Irvine (as of 1 July 1998). Continuing as a collaborator to this effort.
- Dahl, E. E., Member of the Technical Staff, Aeronautics.
- Deusch, S. B., Post-Doctoral Scholar (since 1 May 1998). Continuing the ICV effort and responsible for its extension to 3-D.
- Dimotakis, P. E., John K. Northrop Professor of Aeronautics & Professor of Applied Physics (PI).
- Egolfopoulos, F. N., Associate Professor, Mech. Eng., USC. Also, Visiting Research Associate, Aeronautics, Caltech. Collaborator on chemically-reacting flows and hydrocarbon ignition simulations.
- Lang, D. B., Research Engineer, Aeronautics.
- Leonard, A., Professor, Aeronautics (Co-PI).
- Papalexandris, M. V., originally as Graduate Research Assistant, in Aeronautics at Caltech. Presently with the Jet Propulsion Laboratory (since March 1998).
- Shan, J. W., Graduate Research Assistant, Aeronautics.
- Slessor, M. D., Graduate Research Assistant, Aeronautics. With Allied Signal (Palo Alto, CA), since 1 July 1998.

- Su, Wei-Jen, Graduate Research Assistant, Aeronautics (since 15 June 1998).
- Svitek, P., Staff Engineer.

3.2 Other collaborators

- Cook, A. W., Lawrence Livermore National Laboratory. Collaborator on direct numerical simulations of three-dimensional, variable-density flows.
- Cook, Grant, Lawrence Livermore National Laboratory. Collaborator on direct numerical simulations of variable-density flows and flows with strong fronts.
- Collins, S. A., JPL (digital imaging; KFS effort).
- Elliot, T., JPL (digital imaging; KFS effort).
- Gornowicz, G. G., DreamWorks SKG (Glendale, CA), continuing informal collaborator in our ICV effort.
- Henderson, R., Sr. Research Fellow, Aeronautics and Applied Mathematics, Caltech. Collaborator, with F. Egolfopoulos and D. Meiron, on direct-numerical simulations of 3-D, low Mach number, variable-density, and chemically-reacting flows.
- Kern, Brian, Graduate Research Assistant, Astronomy, Caltech. Collaborator in our high framing-rate imaging (KFS) effort.
- Laidlaw, D. H., Senior Research Fellow, Biology and Computer Science, Caltech. Collaborator on 3-D isosurface computer visualization. Since 1 August 1998, Assistant Professor, Computer Science, Brown University.
- Martin, C., Prof. Physics, Caltech. Collaborator in our high framing-rate imaging (KFS) effort.
- Meiron, D. I., Prof. Applied Mathematics, Caltech. Collaborator, with R. Henderson and F. Egolfopoulos on direct-numerical simulations of 3-D, variable-density flows.
- Miller, P. L., Lawrence Livermore National Laboratory. Collaborator on turbulent mixing in a variety of compressible- and incompressible-turbulence contexts
- Patton, J. M., Member of the Technical Staff, Center for Advanced Computing Research (CACR), Caltech. Collaborator on 3-D computer visualization.

- Vagelopoulos, C. M., Graduate Research Assistant, Mechanical Engineering, USC. Collaboration in extension of Particle-Streak Velocimetry methods in strained flames and hydrocarbon flame-speed measurements.
- Wadsworth, M., JPL (digital imaging). Principal designer of kilo-frame/sec (KFS) CCD focal-plane array.

4. Publications of work supported by this Grant

Reports submitted, accepted, or published of work performed under sponsorship of this grant:

CATRAKIS, H. J. & DIMOTAKIS, P. E. 1998 "Shape Complexity in Turbulence," *Phys. Rev. Lett.* **80**, 968–971.

DIMOTAKIS, P. E., CATRAKIS, H. J., COOK, A. W. & PATTON, J. M. 1998a "On the geometry of two-dimensional slices of irregular level sets in turbulent flows," 2nd *Monte-Verita Colloquium on Fundamental Problematic Issues in Turbulence*, 22–28 March 1998 (Ascona, Switzerland), GALCIT Report FM98–2.

DIMOTAKIS, P. E., CATRAKIS, H. J. & FOURGUETTE, D. C. 1998b "Beam Propagation and Phase-Front Integrals in High Reynolds Number Shear Layers and Jets," *AIAA* 29th *Plasmadynamics and Lasers Conference*, Paper 98–2833.

EGOLFOPOULOS, F. N. & DIMOTAKIS, P. E. 1998 "Non-premixed hydrocarbon ignition at high strain rates," *Twenty-Seventh Symposium (International) on Combustion*, Paper 5C11. GALCIT Report FM98–7.

LAPPAS, T., LEONARD, A. & DIMOTAKIS, P.E. 1998 "Riemann invariant manifolds for the multidimensional Euler equations," *SIAM J. Sci. Comp.* (accepted).

SLESSOR, M. D. 1998 *Aspects of turbulent-shear-layer dynamics and mixing*, Ph.D. thesis, California Institute of Technology.

SLESSOR, M. D., BOND, C. L. & DIMOTAKIS, P. E. 1998 "Turbulent shear-layer mixing at high Reynolds numbers: effects of inflow conditions," *J. Fluid Mech.* (accepted). GALCIT Report FM98–1.

SLESSOR, M. D., ZHUANG, M. & DIMOTAKIS, P. E. 1998 "Turbulent shear-layer mixing: growth-rate compressibility scaling," GALCIT Report FM98–9.

5. Interactions/Transitions

Visits/interactions/participation/presentations at meetings, conferences, seminars:

- Bond (presenter), C. L., "Mixing in high Reynolds number shear layers." GALCIT Fluid Mechanics Seminar (6 March 1998).
- Catrakis (presenter), H. J., and Bond, C. L., "Scale distributions of geometric transects of level sets," contributed presentation, Am. Phys. Soc., Div. Fluid Dynamics, annual meeting (San Francisco, CA, November 1997).
- Dimotakis (presenter), P. E., "Turbulence, fractals, and mixing." Plenary lecture, Am. Phys. Soc., Div. Fluid Dynamics, annual meeting (San Francisco, CA, November 1997).
- Papalexandris (presenter), M. V., Leonard, A., and Dimotakis, P. E., "Unsplit Schemes for Multi-Dimensional Systems of Hyperbolic Conservation Laws with Source Terms," contributed presentation, Am. Phys. Soc., Div. Fluid Dynamics, annual meeting (San Francisco, CA, November 1997).
- Shan (presenter), J. W., Laidlaw, D. H., Gornowicz, G. G., Lang, D. B., and Dimotakis, P. E., "Three-Dimensional Space-Time Structure of Turbulent Jets," contributed presentation, Am. Phys. Soc., Div. Fluid Dynamics, annual meeting (San Francisco, CA, November 1997).
- Slessor (presenter), M. D., Bond, C. L., and Dimotakis, P. E., "The effect of initial conditions on turbulent shear layers," contributed presentation, Am. Phys. Soc., Div. Fluid Dynamics, annual meeting (San Francisco, CA, November 1997).
- Dimotakis (presenter), P. E., "Image correlation velocimetry and the flow over an accelerating NACA–0012 airfoil." GALCIT Fluid Mechanics Seminar, with R. Henderson (9 January 1998).
- Slessor (presenter), M. D., "Dynamics and Mixing of Turbulent Shear layers." GALCIT Fluid Mechanics Seminar (6 March 1998).

- Dimotakis (presenter), P. E., Catrakis, H. J., Cook, A. W., and Patton, J. M., "On the geometry of two-dimensional slices of irregular level sets in turbulent flows." Invited lecture, 2nd *Monte Verita Colloquium on Fundamental Problematic Issues in Turbulence* (22–28 March 1998, Ascona, Switzerland).
- Dimotakis (presenter), P. E., and Slessor, M. D., "Mixing in high Reynolds number shear layers." Plenary lecture, AIAA Fluid Dynamics meeting (Albuquerque, NM, June 1998).
- Egolfopoulos (presenter), F. N., and Dimotakis, P. E., "Effects of additives on hydrocarbon ignition at high strain rates." 27th International Combustion Symposium presentation/paper (Boulder, CO, August 1998).
- Clavin (U. Marseilles), Paul: Discussions on detonation, supersonic test facilities, and related research issues (August 1998 visit to Caltech).

Consultative and advisory functions to other labs, agencies, especially AF and DoD (include institutions, locations, dates, names):

- Dimotakis, P. E., Lawrence Livermore National Laboratories. Consulting on compressible turbulence, inertial-confinement fusion, high-fluence laser-doubling crystal growth (1993 to present).
- Dimotakis, P. E., Member of NAS/NRC Committee that reviewed DOE's Inertial Confinement Fusion (ICF) program and the National Ignition Facility (work completed August 1997).
- Dimotakis, P. E., Member Mitre/JASON group.

Transitions (cases where knowledge resulting from this research is used or will be used in a technology application):

- None

New Discoveries, inventions, patents:

- None